

Heat Conduction in Ceramic Coatings: Relationship between Microstructure and Effective Thermal Conductivity

Technical report for Task 2 (Second Year)

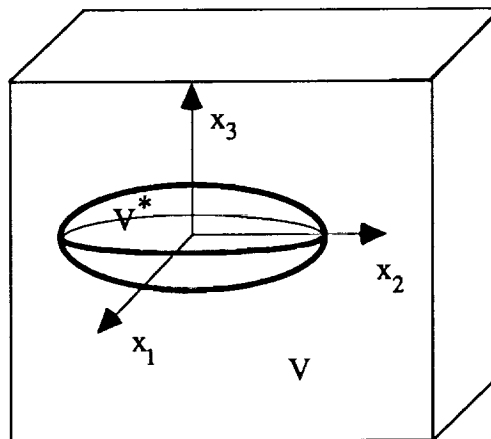
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Analysis of the effective thermal conductivity of ceramic coatings and its relation to the microstructure continued. Results (obtained in Task 1) for the three-dimensional problem of heat conduction in a solid containing an inclusion (or, in particular, cavity - thermal insulator) of the ellipsoidal shape, were further advanced in the following two directions:

- closed form expressions of H tensor have been derived for special cases of ellipsoidal cavity geometry: spheroid, crack-like spheroidal cavity and needle shaped spheroidal cavity;
- these results for one cavity have been incorporated to contrast heat energy potential for a solid with many spheroidal cavities (in the approximation of non-interacting defects).

This problem constitutes a basic building block for further analyses, since the ellipsoidal shape covers a variety of practically important pore geometries.



The problem is formulated as the determination of the change in thermal conductivity due to inclusion. Namely:

$$\Delta Q = H \cdot G \quad (1)$$

where ΔQ is the heat flux change per reference volume V , G is the far-field temperature gradient and second rank tensor H is a function of the inclusion shape and the inclusion conductivity.

Mathematical considerations based on the analysis of the ellipsoidal shapes in the framework of Eshelby-type theory and on utilization of Green's function for the heat conduction problem in an unbounded medium, show that H has the following form:

$$H = \frac{V^*}{V} (k_* - k_0) (A_1 I + A_2 mm + A_3 nn) \quad (2)$$

where $V^* = \frac{4\pi}{3} a_1 a_2 a_3$ is the volume of the ellipsoidal inclusion with semi-axes a_1, a_2, a_3 with unit vectors I, m, n ; k_* and k_0 are conductivities of the inclusion and of the matrix, correspondingly. Coefficients A_1, A_2, A_3 are given in terms of elliptic integrals (see Report for Task 1).

In the case when the inclusion is a *spheroid* ($a_1 = a_2 \equiv a$), tensor H takes the form

$$H = \frac{V^*}{V} (k_* - k_0) \left\{ \left[1 + \frac{k_* - k_0}{k_0} f_0(\gamma) \right]^{-1} (I - nn) + \left[1 + \frac{k_* - k_0}{k_0} (1 - 2f_0(\gamma)) \right]^{-1} nn \right\} \quad (3)$$

or, in components:

$$H_{ij} = \frac{V^*}{V} (k_* - k_0) \left\{ \left[1 + \frac{k_* - k_0}{k_0} f_0(\gamma) \right]^{-1} (\delta_{ij} - n_i n_j) + \left[1 + \frac{k_* - k_0}{k_0} (1 - 2f_0(\gamma)) \right]^{-1} n_i n_j \right\} \quad (4)$$

where it is denoted:

$\gamma = a/a_3$ - aspect ratio of the spheroidal inclusion,

$n = n_1 e_1 + n_2 e_2 + n_3 e_3$ - unit vector along the axis of symmetry of spheroid,

$I = e_1 e_1 + e_2 e_2 + e_3 e_3$ - unit second rank tensor,

$$f_0(\gamma) = \frac{1 - g(\gamma)}{2(1 - \gamma^2)}, \quad g(\gamma) = \frac{\gamma^2}{\sqrt{\gamma^2 - 1}} \arctan \sqrt{\gamma^2 - 1} \quad (\text{for oblate shape, } \gamma > 1),$$

$$g(\gamma) = \frac{\gamma^2}{2\sqrt{1 - \gamma^2}} \ln \frac{1 + \sqrt{1 - \gamma^2}}{1 - \sqrt{1 - \gamma^2}} \quad (\text{for prolate shape, } \gamma < 1).$$

- In the case of *spheroidal cavity* (insulator, $k_* = 0$) tensor \mathbf{H} is as follows:

$$\mathbf{H} = -\frac{V^*}{V} k_0 \left\{ \frac{1}{1 + f_0(\gamma)} (\mathbf{I} - \mathbf{nn}) + \frac{1}{2f_0(\gamma)} \mathbf{nn} \right\} \quad (5)$$

- In the case of *thin spheroidal cavity* ($\gamma \gg 1$):

$$\mathbf{H} = -\frac{V^*}{V} k_0 \left\{ \frac{1}{1 + \pi/(4\gamma)} (\mathbf{I} - \mathbf{nn}) + \frac{2\gamma}{\pi} \mathbf{nn} \right\} \quad (6)$$

- In the limit of a *circular crack* :

$$\mathbf{H} = -\frac{8a^3}{3V} k_0 \mathbf{nn} \quad (7)$$

- In the case of *needle-shaped spheroidal cavity* ($\gamma \ll 1$):

$$\mathbf{H} = -\frac{V^*}{V} k_0 \left\{ \left[1 - \frac{1}{2} \left(1 + \gamma^2 - \gamma^2 \ln \frac{2}{\gamma} \right) \right]^{-1} (\mathbf{I} - \mathbf{nn}) + \left(1 + \gamma^2 - \gamma^2 \ln \frac{2}{\gamma} \right) \mathbf{nn} \right\} \quad (8)$$

In the approximation of non-interacting cavities (each cavity experiences the influence of the same far-field temperature gradient \mathbf{G} unperturbed by the presence of other cavities), the *heat energy potential* $\Delta\Omega$ for a solid with many cavities is obtained as follows (in terms of derived tensors $\mathbf{H}^{(i)}$ characterizing i -th cavity):

$$\Delta\Omega = \frac{1}{2} \mathbf{G} \cdot \left[\sum_i \mathbf{H}^{(i)} \right] \cdot \mathbf{G} \quad (9)$$

For example, in the case of *spherical* cavities we have:

$$\sum_i \mathbf{H}^{(i)} = -\frac{3}{2} k_0 \mathbf{I} \left[\frac{1}{V} \sum_i V^{*(i)} \right] = -\frac{3}{2} p k_0 \mathbf{I} \quad (10)$$

$$\Delta\Omega = -\frac{3}{4} p k_0 \mathbf{G} \cdot \mathbf{G} = -\frac{3}{4} p k_0 (G_1^2 + G_2^2 + G_3^2) \quad (10a)$$

where parameter p is the conventional porosity.

In the case of *circular cracks* we have:

$$\sum_i H^{(i)} = -\frac{8}{3}k_0 \left[\frac{1}{V} \sum_i (a^3 nn)^{(i)} \right] = -\frac{8}{3}k_0 \alpha \quad (11)$$

$$\Delta \Omega = -\frac{4}{3}k_0 \mathbf{G} \cdot \boldsymbol{\alpha} \cdot \mathbf{G} \quad (11a)$$

where $\boldsymbol{\alpha}$ is the second rank crack density tensor (well known in problems of effective *elastic* properties of cracked media).

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